

Correlation Trends in the Hyperfine Structures of $^{210,212}\text{Fr}$

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We demonstrate the importance of electron correlation effects in the hyperfine structure constants of many low-lying states in ^{210}Fr and ^{212}Fr . This is achieved by calculating the magnetic dipole and electric quadrupole hyperfine structure constants using the Dirac-Fock approximation, second order many-body perturbation theory and the coupled-cluster method in the singles and doubles approximation in the relativistic framework. By combining our recommended theoretical results with the corresponding experimental values, improved nuclear magnetic dipole and electric quadrupole moments of the above isotopes are determined. In the present work, it is observed that there are large discrepancies between the hyperfine structure constants of the $7D_{5/2}$ state obtained from the experimental and theoretical studies whereas good agreements are found for the other $D_{5/2}$ states. Our estimated hyperfine constants for the $8P$, $6D$, $10S$ and $11S$ states could be very useful as benchmarks for the measurement of these quantities.

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I. INTRODUCTION

Francium (Fr) is the heaviest alkali atom in the periodic table possessing 87 electrons. Therefore, the properties of this system are expected to exhibit moderately strong correlation effects, and their determination calls for using powerful many-body methods. Like other alkali atoms, Fr atom is also being considered for many important experimental studies, prominent among them being the measurement of the electric dipole moment (EDM) due to parity and time reversal symmetries [1, 2] and parity nonconservation (PNC) effects due to neutral weak interaction [2, 3] and the nuclear anapole moment [4] owing to its relatively heavy size. Like the EDM and PNC interactions, the magnetic dipole hyperfine interaction has a fairly strong dependence on Z , the atomic number of the system [5] as it involves an electron interacting with the nucleus. Thus, theoretical investigations of hyperfine structures are necessary for EDM and PNC studies to test the accuracies of the wave functions in the nuclear region [6, 7]. On the other hand, comparison of theoretical results from various approximations with the experimental values can provide a comprehensive understanding of the passage of electron correlations from lower to higher levels of many-body theory. This knowledge is essential to validate the theoretical results when the experimental values are unavailable. Attempts have been made to investigate trends in the correlation effects in the calculations of hyperfine structure constants of the S -states using lower order many-body methods [8–11], but such trends have not been demonstrated explicitly for states having higher angular momentum in Fr.

Here, we intend to show the variation in the trends of

correlation effects in the evaluation of hyperfine structure constants of as many as 17 low-lying states in Fr considering relativistic second order many-body perturbation theory (MBPT(2) method) and the coupled-cluster (CC) method at various levels of approximation using the reference states obtained by the Dirac-Fock (DF) method with V^{N-1} potential. In the present work, we have undertaken theoretical studies of the hyperfine structure constants of ^{210}Fr and ^{212}Fr isotopes for two reasons. First, ^{210}Fr has been proposed as one of the most suitable Fr isotopes for both the PNC and EDM studies [1, 2]. To draw meaningful conclusions and to be consistent in the findings from comparisons between the theoretical and experimental hyperfine structure constants of different states, it is necessary to consider the results for as many as states as possible for both the isotopes. The second, but the essential reason behind considering the above two isotopes is that experimental results of hyperfine structure constants for only a few selective low-lying states of ^{210}Fr [12–15] and some other excited states of ^{212}Fr are available [16].

II. THEORY

The Hamiltonian describing non-central form of hyperfine interaction between the electrons and nucleus in an atomic system is expressed in terms of tensor operator products as [17]

$$H_{hf} = \sum_k \mathbf{M}_n^{(k)} \cdot \mathbf{O}_{hf}^{(k)}, \quad (1)$$

where $\mathbf{M}_n^{(k)}$ and $\mathbf{O}_{hf}^{(k)}$ are the spherical tensor operators with rank k (> 0) in the nuclear and electronic coordinates respectively. Since these interaction strengths become much weaker with higher values of k , we consider only up to $k = 2$ for the present case. Due to the

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coupling between the electronic (J) and nuclear (I) angular momentums, $|\gamma IJ; FM_F\rangle$ states are the proper bases with total angular momentum $\mathbf{F} = \mathbf{J} + \mathbf{I}$ and corresponding azimuthal quantum number M_F and γ representing rest of the unspecified quantum numbers.

The energy splitting due to first order correction in the atomic state $|JM\rangle$ because of the hyperfine interaction is given by

$$\begin{aligned} W_{F,J}^{(1)} &= \langle \gamma IJ; FM_F | \sum_k \mathbf{M}_n^{(k)} \cdot \mathbf{O}_{hf}^{(k)} | \gamma IJ; FM_F \rangle \\ &= \sum_k (-1)^{I+J+F} \begin{Bmatrix} J & I & F \\ I & J & k \end{Bmatrix} \\ &\quad \times \langle I || M_n^{(k)} || I \rangle \langle J || O_{hf}^{(k)} || J \rangle \end{aligned} \quad (2)$$

which after expanding up to multipoles $k = 2$, we get

$$W_{F,J}^{(1)} = W_{F,J}^{M1} + W_{F,J}^{E2}, \quad (3)$$

where $W_{F,J}^{M1}$ and $W_{F,J}^{E2}$ are the contributions due to the magnetic dipole (M1) with $k = 1$ and electric quadrupole (E2) with $k = 2$ interactions respectively. Traditionally it is expressed as

$$W_{F,J}^{M1} = \frac{1}{2} A_{hf} K \quad (4)$$

and

$$W_{F,J}^{E2} = B_{hf} \frac{\frac{3}{4}K^2 + \frac{3}{4}K - I(I+1)J(J+1)}{2I(2I-1)J(2J-1)} \quad (5)$$

with the hyperfine structure constants defined as

$$A_{hf} = \mu_N g_I \frac{\langle J || O_{hf}^{(1)} || J \rangle}{\sqrt{J(J+1)(2J+1)}} \quad (6)$$

and

$$\begin{aligned} B_{hf} &= 2Q \left[\frac{2J(2J-1)}{(2J+1)(2J+2)(2J+3)} \right]^{1/2} \\ &\quad \times \langle J || O_{hf}^{(2)} || J \rangle, \end{aligned} \quad (7)$$

where μ_N is the nuclear Bohr magneton, $g_I = \frac{\mu_I}{I}$, μ_I and Q are the nuclear magnetic and quadrupole moments respectively, and $K = F(F+1) - I(I+1) - J(J+1)$. It appears from the above expressions that the quantities A_{hf}/g_I and B_{hf}/Q are independent of nuclear factors, but these values can slightly vary among isotopes due to different nuclear potentials seen by electrons in these systems.

III. METHOD OF CALCULATIONS

In the Block's equation formalism, atomic wave function ($|\Psi_n\rangle$) of any of the considered states with closed-shell configuration $[6p^6]$ and a respective valence orbital n in Fr can be expressed as [18]

$$|\Psi_n\rangle = \Omega_n |\Phi_n\rangle, \quad (8)$$

where Ω_n is known as the wave operator that generates virtual excitations from the reference state $|\Phi_n\rangle$ to form all possible excited configurations to give rise the exact state $|\Psi_n\rangle$. The choice of $|\Phi_n\rangle$ can be crucial in obtaining accurate results, but we construct it using V^{N-1} potential by expressing $|\Phi_n\rangle = a_n^\dagger |\Phi_0\rangle$ with DF wave function $|\Phi_0\rangle$ of the closed-core $[6p^6]$ obtained by considering the Dirac-Coulomb (DC) Hamiltonian (H_{DC}) and is the working reference state for all the considered atomic states.

To account for the electron correlation effects through Ω_n in the evaluation of $|\Psi_n\rangle$, we proceed in two successive steps. In the first step, we consider correlation effects within the closed-shell configuration $[6p^6]$, following which we take into account correlation of the valence electron coupling with the core electrons to generate the virtual excitations. For this purpose, we express Ω_n as

$$\Omega_n = \Omega_0 + \Omega_n^v, \quad (9)$$

where Ω_0 (independent of n) takes care of correlation effects from the closed-core while Ω_n^v is responsible for incorporating correlation corrections involving the electron from the valence orbital. In the perturbative expansion, we write [18]

$$\Omega_n = \sum_{k=0}^2 \Omega_n^{(k)} \quad (10)$$

with $\Omega_n^{(k)}$ corresponds to wave operator with presence of k number of Coulomb interaction operator in it. The hyperfine structure constants in this method are determined by calculating the reduced matrix elements of the $O_{hf}^{(1)}$ and $O_{hf}^{(2)}$ operators (below denoted simply by O) using the following expression

$$\begin{aligned} \frac{\langle \Psi_n | O | \Psi_n \rangle}{\langle \Psi_n | \Psi_n \rangle} &= \frac{\langle \Phi_n | \Omega_n^\dagger O \Omega_n | \Phi_n \rangle}{\langle \Phi_n | \Omega_n^\dagger \Omega_n | \Phi_n \rangle} \\ &= \frac{\langle \Phi_n | \sum_{i,j} \Omega_n^{(i)\dagger} O \Omega_n^{(j)} | \Phi_n \rangle}{\langle \Phi_n | \sum_{i,j} \Omega_n^{(i)\dagger} \Omega_n^{(j)} | \Phi_n \rangle}. \end{aligned} \quad (11)$$

For the MBPT(2) method, $i + j \leq 2$ in the above summations.

In the Fock space CC approach, we define $\Omega_0 = e^T$ and $\Omega_n^v = e^T S_n$ that yields the form

$$|\Psi_n\rangle = e^T \{1 + S_n\} |\Phi_n\rangle, \quad (12)$$

where T and S_n are the excitation operators involving core and core-valence electrons respectively. Since our reference state is $|\Phi_0\rangle$, we take S_v in normal order with respect to $|\Phi_0\rangle$ which, here, has been denoted by $\{S_n\}$. It is worthwhile to mention that T is also in normal order with respect to $|\Phi_0\rangle$ by construction. From a practical point of view we only consider the singles and doubles excitations through the CC operators, known as the CCSD method in the literature [19, 20], by defining

$$T = T_1 + T_2 \quad \text{and} \quad S_n = S_{1n} + S_{2n}. \quad (13)$$

Even though the CC operators have been approximated, we are able to account many important contributions from the triples and quadruples through the non-linear terms of Eq. (12). In order to understand role of these contributions in Fr for accurate evaluation of its hyperfine structure constants, we also determine contributions only considering the linear terms of Eq. (12) by approximating

$$|\Psi_n\rangle = \{1 + T_1 + T_2 + S_{1n} + S_{2n}\}|\Phi_n\rangle, \quad (14)$$

which we refer to as LCCSD method. One more remark on this approximation is that it resembles the form of the singles and doubles configuration interaction (CISD) method.

The hyperfine structure constants are determined in the CC method as

$$\frac{\langle\Psi_n|O|\Psi_n\rangle}{\langle\Psi_n|\Psi_n\rangle} = \frac{\langle\Phi_n|\{1 + S_n^\dagger\}e^{T^\dagger}Oe^T\{1 + S_n\}|\Phi_n\rangle}{\langle\Phi_n|\{1 + S_n^\dagger\}e^{T^\dagger}e^T\{1 + S_n\}|\Phi_n\rangle}. \quad (15)$$

The above expression has two non-truncative series $e^{T^\dagger}Oe^T$ and $e^{T^\dagger}e^T$ in the numerator and denominator respectively. To account for the contributions that are significant from these series, we have used the Wick's general theorem to divide these terms into effective one-body, two-body and three-body terms [18]. The effective one-body terms are dominant owing to the single particle form of the above O operators, they are computed self-consistently and stored as intermediate parts before contracting with the corresponding S_n operators. While the effective two-body and three-body terms are computed directly, but we also reuse the effective one-body terms to construct the effective two-body and three-body terms. To give an illustrate example of the adopted computational procedure in our calculations, we outline the important steps below. In the first step, we calculate the effective one-body terms of $e^{T^\dagger}e^T$ and store them as hole-hole (H-H), particle-particle (P-P), and particle-hole (P-H) blocks. The P-H block is first evaluated considering only linear terms and then stored as an intermediate effective P-H block which then contracted further with an extra T_2^\dagger operator to get the H-P block. Consequently, the P-H block is obtained from the H-P block by multiplying appropriate phase factors and the procedure is repeated till the self-consistent results with tolerance size 10^{-8} achieved. Following this, the H-H and P-P blocks are constructed considering the direct contractions among the T_2 and T_2^\dagger operators and along with the contractions of the H-P and H-P blocks with the T_1 operators. As a result, the H-H and P-P blocks still contain terms from infinite series through the H-P and P-H blocks. In a similar fashion we compute $e^{T^\dagger}Oe^T$ but by slightly modifying the above strategy. Here we make use of the effective one-body terms of $e^{T^\dagger}e^T$ for the construction of the effective one-body diagrams of $e^{T^\dagger}Oe^T$ and special attention has been paid to avoid the repetition

TABLE I: List of different parameters of bases used in the present calculations.

	s	p	d	f	g
N_l	40	39	38	37	36
α_0	2.0×10^{-8}	2.5×10^{-8}	2.5×10^{-8}	2.1×10^{-1}	2.1×10^{-7}
β	5.06	5.04	5.06	5.08	5.15

of any diagram through the iterative procedure. We also replaced the T_1 and its conjugate operators appearing in the effective two-body and three-body terms of $e^{T^\dagger}Oe^T$ by the effective P-H block and H-P block of $e^{T^\dagger}e^T$ to improve the results with the contributions from higher order CC terms.

We also estimate contributions from the important triple excitations considering them perturbatively in the above property evaluation expression by defining a triple excitation operator

$$S_{3n}^{pert} = \frac{1}{4} \sum_{ab,pqr} \frac{(H_{DC}T_2 + H_{DC}S_{2n})_{abn}^{pqr}}{\epsilon_n + \epsilon_a + \epsilon_b - \epsilon_p - \epsilon_q - \epsilon_r}, \quad (16)$$

where a, b and p, q, r indices represent for core and virtual orbitals respectively. Particles appearing in the subscripts are annihilated while those appear in the superscripts are created in the course of defining excitation processes. We refer to this approach as the CCSD_{t3} method in this work.

We use a recently developed basis function having the analytic exponential form with quadratic exponents to express the single particle wave functions. These functions for the orbitals having orbital angular momentum value l are given as

$$|\phi^l(r)\rangle = r^l \sum_{\nu=1}^{N_l} c_\nu^l e^{-\alpha_\nu r^4} |\chi(\theta, \varphi)\rangle, \quad (17)$$

where $|\chi(\theta, \varphi)\rangle$ represents the angular momentum part, N_l corresponds to the total number of analytic functions considered in the calculations and α_ν is an arbitrary coefficient constructed satisfying the even tempering condition between two parameters α_0 and β as

$$\alpha_\nu = \alpha_0 \beta^{\nu-1}. \quad (18)$$

The motive for using the above analytic function is to describe the atomic wave functions more accurately in the nuclear region of a heavy atom like Fr than the Slater and Gaussian type orbitals. We give the list of parameters in Table I used in the present calculations.

IV. RESULTS AND DISCUSSION

In order to demonstrate the propagation of electron correlation effects from the lower to higher orders of

TABLE II: Results for A_{hf}/g_I and B_{hf}/Q (both are in MHz) obtained using the DF, MBPT(2), LCCSD, CCSD and CCSD_{t3} methods. Previously reported calculations using varieties of many-body methods are also quoted as “Others”.

State	A_{hf}/g_I values						B_{hf}/Q values					
	DF	MBPT(2)	LCCSD	CCSD	CCSD _{t3}	Others	DF	MBPT(2)	LCCSD	CCSD	CCSD _{t3}	Others
$7s\ ^2S_{1/2}$	6531.06	10186.68	11457.29	9916.20	9885.24	9927.69 ^a 9947.07 ^b 10155.40 ^c 8432.65 ^d						
$7p\ ^2P_{1/2}$	707.70	1169.41	1522.50	1281.84	1279.56	1308.67 ^b 1265.77 ^c 876.12 ^e						
$7p\ ^2P_{3/2}$	55.68	97.20	124.80	104.34	104.28	103.38 ^b 115.09 ^c 96.28 ^e	118.03	234.51	300.47	258.99	259.73	231 ^e
$6d\ ^2D_{3/2}$	36.24	44.10	123.00	85.02	85.20		26.19	73.47	100.17	96.33	98.61	
$6d\ ^2D_{5/2}$	14.28	-23.04	-84.36	-58.92	-58.82		30.34	97.09	134.01	129.38	131.40	
$8s\ ^2S_{1/2}$	1674.12	2234.40	2337.92	2159.16	2151.90	2160.98 ^a 2165.88 ^b 2218.47 ^c 2155.27 ^d						
$8p\ ^2P_{1/2}$	251.76	381.06	457.38	402.84	402.01	408.68 ^b 409.46 ^c						
$8p\ ^2P_{3/2}$	20.40	33.96	40.62	35.04	35.03	34.25 ^b 39.64 ^c	43.29	78.74	94.73	83.81	84.01	
$7d\ ^2D_{3/2}$	18.30	16.14	36.45	30.84	30.90		13.23	24.99	29.28	29.97	30.53	
$7d\ ^2D_{5/2}$	6.90	-12.24	-18.62	-16.32	-16.28		14.57	32.84	38.56	39.45	39.92	
$9s\ ^2S_{1/2}$	687.54	881.28	910.01	852.78	849.72	852.39 ^a 839.40 ^d						
$10s\ ^2S_{1/2}$	382.38	468.12	449.63	455.82	454.26	402.97 ^d						
$8d\ ^2D_{3/2}$	9.38	7.75	16.62	14.45	14.47		6.79	9.47	13.15	13.43	13.66	
$8d\ ^2D_{5/2}$	3.46	-5.34	-7.62	-6.90	-6.88		7.35	12.62	17.26	17.59	17.78	
$9d\ ^2D_{3/2}$	5.08	4.22	9.13	7.84	7.86		3.68	5.01	7.08	7.12	7.24	
$9d\ ^2D_{5/2}$	1.87	-3.02	-3.89	-3.53	-3.52		3.96	6.74	9.21	9.25	9.35	
$11s\ ^2S_{1/2}$	186.13	238.72	252.16	231.13	230.12	208.11 ^d						

^a[15], ^b[21], ^c[22], ^d[11], ^e[23].

many-body methods, we present results using the DF, MBPT(2), LCCSD, CCSD and CCSD_{t3} methods for A_{hf}/g_I and B_{hf}/Q of the first 17 low-lying states of ²¹⁰Fr in Table II. We find changes beyond third decimal places in these results for all the states except for the A_{hf}/g_I values of the s -states, which are reduced by -1.141, -0.242, -0.095, -0.047 and -0.028 (in MHz) in the $7S$, $8S$, $9S$, $10S$ and $11S$ states, respectively, of ²¹²Fr compared to the results of ²¹⁰Fr. We account for these differences later while considering the results for ²¹²Fr. It can be seen from the above table that the MBPT(2) results are larger than the corresponding DF results for

both the properties except for the A_{hf}/g_I values of the $D_{5/2}$ states. In fact, there are sign differences between the DF and MBPT(2) results of A_{hf}/g_I in the $D_{5/2}$ states implying that correlation effects are very strong for these states. It is found that the LCCSD method yields much larger values for both A_{hf}/g_I and B_{hf}/Q compared to the other methods. The non-linear terms in the CCSD methods contribute substantially but with opposite sign to reduce the LCCSD values. Triples through the CCSD_{t3} method also further reduce the A_{hf}/g_I values while they lead to small increases in the values of B_{hf}/Q . Thus, we conclude that the correlations effects

TABLE III: Contributions from individual LCCSD and CCSD terms to the A_{hf}/g_I calculations in the $7S$, $7P$, $6D$ and $8S$ states (in MHz). *Extra* and *norm* correspond to contributions from the non-linear terms of the CCSD method that are not mentioned explicitly and corrections due to the normalization of the wave functions respectively. *cc* means complex conjugate.

CC term	$7s\ ^2S_{1/2}$		$7p\ ^2P_{1/2}$		$7p\ ^2P_{3/2}$		$6d\ ^2D_{3/2}$		$6d\ ^2D_{5/2}$		$8s\ ^2S_{1/2}$	
	LCCSD	CCSD	LCCSD	CCSD	LCCSD	CCSD	LCCSD	CCSD	LCCSD	CCSD	LCCSD	CCSD
$OT_1 + cc$	-440.401	-437.580	-11.058	-18.540	-1.050	-1.740	0.150	0.042	0.108	0.066	-101.161	-101.52
$T_1^\dagger OT_1$	7.422	7.326	0.042	0.120	0.006	0.014	~ 0	~ 0	~ 0	~ 0	1.524	1.536
$T_1^\dagger OT_2$	-17.701	-19.321	-0.486	-1.260	0.010	0.018	~ 0	-0.002	-0.002	0.002	-4.092	-4.230
$T_2^\dagger OT_2$	-72.300	-75.721	-4.548	-5.628	1.848	1.920	1.230	1.068	2.202	2.226	-16.356	-16.548
$OS_{1v} + cc$	3684.661	2821.14	486.901	363.721	31.956	23.388	57.438	36.888	18.901	12.198	494.341	389.70
$OS_{2v} + cc$	1363.981	1059.001	225.720	175.620	28.698	20.100	-5.064	-4.518	-96.420	-70.021	308.040	246.00
$T_1^\dagger OS_{2v} + cc$	-36.96	-42.801	-3.150	-3.498	-0.204	-0.228	-0.396	-0.384	-0.144	-0.138	-4.320	-10.098
$T_2^\dagger OS_{2v} + cc$	-227.890	-191.930	-0.180	-0.174	0.099	-0.060	0.228	0.126	0.168	0.036	-47.240	-40.91
$S_{1v}^\dagger OS_{1v}$	519.661	304.620	83.821	46.758	4.590	2.460	22.962	9.462	6.300	2.544	36.486	22.680
$S_{1v}^\dagger OS_{2v} + cc$	288.301	178.501	53.310	32.268	5.412	2.976	3.498	1.014	-47.280	-23.706	18.186	13.518
$S_{2v}^\dagger OS_{2v}$	353.880	225.481	31.326	21.690	0.570	0.618	23.358	13.482	8.724	4.476	74.580	49.398
<i>Extra</i>		-90.476		-12.198		0.522		-2.022		-2.208		-56.382
<i>norm</i>	-495.831	-267.311	-46.836	-24.738	-2.604	-1.326	-16.596	-6.378	8.778	3.072	-91.911	-46.723

represented by the non-linear terms that correspond to triple and quadruple excitations are crucial for the accurate evaluation of the hyperfine structure constants in Fr atom.

We also mention about previously reported calculations of A_{hf}/g_I and B_{hf}/Q in Fr in Table II as “Others” [11, 15, 21–23]. Owusu et al. had investigated the core-polarization effects systematically in the S - states of ^{212}Fr using relativistic many-body perturbation theory equivalent to our MBPT(2) method. These values are found to be smaller than our MBPT(2) results. SDpT method, analogous to our LCCSD approximation but with important triples effects in the wave function determination, has been employed in Refs. [15, 21] to evaluate the A_{hf}/g_I values of a few low-lying states and are in close agreement with our CCSD and CCSD $_{t3}$ results. Dzuba et al had employed a restricted Hartree-Fock method in the relativistic framework and incorporated correlation effects using many-body perturbation theory to investigate correlation effects in the hyperfine structure constants of a few low-lying states of ^{211}Fr [22]. Heully and Mårtensson-Pendrill had employed a relativistic many-body perturbation method treating polarization effects to all orders. Their results differ [23] significantly from our calculations.

Having demonstrated that substantial correlation effects arise through the non-linear terms of the CCSD method above, it would be interesting to know whether these terms are more important for the accurate determination of atomic wave functions which are necessary for PNC and EDM studies in Fr atom or the non-linear terms appearing in Eq. (15). In case of the second possibility, it would be advisable to avoid large scale computations in

the evaluation of the amplitudes of the CC excitation operators. For this reason, we compare contributions arising term by term of Eq. (15) in the LCCSD and CCSD methods. These values for A_{hf}/g_I are given in Tables III, IV and V for each considered state of ^{210}Fr atom. Similarly, the calculated B_{hf}/Q values are given in Tables VI and VII. Comparing contributions from individual terms of LCCSD and CCSD methods, we find the CC amplitudes are substantially changed by the correlation effects through the non-linear terms in the CCSD method. In fact, changes in the results due to normalization of the wave functions in both the methods (given as *norm* in the above tables) are also quite large. Contributions given as *Extra* are from the non-linear terms appearing in Eq. (15) and found to be comparatively small. Clearly, the consideration of non-linear terms of the CCSD method in the calculations of atomic wave functions are very crucial, and they should be considered for obtaining high precision results and are very important for calculating quantities related to EDM and PNC studies in Fr. Even though Eq. (15) contains non-truncative series in the CCSD method, the linear terms contribute dominantly and are mainly responsible for determining the accuracies of the final results.

To understand the role of various correlation effects in the states belonging to different angular momenta, we discuss here the trends in the results through various CC terms for both the LCCSD and CCSD methods. It can be seen from these tables that maximum contribution to A_{hf}/g_I come from OS_{1v} and its complex conjugate (*cc*) terms, which correspond to all order pair-correlation effects [6, 24], followed by $OS_{2v} + cc$ terms, which represent the all order core-polarization effects [6, 24], in the S ,

TABLE IV: Contributions from individual LCCSD and CCSD terms to the A_{hf}/g_I calculations in the $8P$, $7D$, $9S$ and $10S$ states (in MHz). *Extra* and *norm* correspond to contributions from the non-linear terms of the CCSD method that are not mentioned explicitly and corrections due to the normalization of the wave functions respectively.

CC term	$8p\ ^2P_{1/2}$		$8p\ ^2P_{3/2}$		$7d\ ^2D_{3/2}$		$7d\ ^2D_{5/2}$		$9s\ ^2S_{1/2}$		$10s\ ^2S_{1/2}$	
	LCCSD	CCSD	LCCSD	CCSD	LCCSD	CCSD	LCCSD	CCSD	LCCSD	CCSD	LCCSD	CCSD
$OT_1 + cc$	-3.090	-6.198	-0.264	-0.564	0.084	0.036	0.054	0.036	-40.098	-40.410	-19.895	-20.096
$T_1^\dagger OT_1$	0.096	0.036	0.001	0.001	~ 0	~ 0	~ 0	~ 0	0.582	0.594	0.285	0.291
$T_1^\dagger OT_2 + cc$	0.138	-0.276	0.001	0.003	~ 0	-0.001	-0.001	-0.001	-1.626	-1.680	-0.807	-0.833
$T_2^\dagger OT_2$	-1.764	-0.252	1.164	0.942	0.720	0.540	1.032	0.972	-7.476	-7.524	-3.846	-3.872
$OS_{1v} + cc$	121.861	93.060	8.670	6.468	11.700	8.646	3.606	2.610	162.780	128.701	74.151	60.405
$OS_{2v} + cc$	71.940	9.510	9.666	7.008	1.524	0.762	-31.716	-25.458	122.341	98.400	60.806	49.144
$T_1^\dagger OS_{2v} + cc$	-1.074	-1.212	-0.072	-0.084	-0.150	-0.156	-0.126	-0.054	-3.504	-4.080	-1.761	-2.051
$T_2^\dagger OS_{2v} + cc$	-0.540	-0.060	-0.036	-0.018	0.078	0.048	0.054	0.030	-18.321	-15.962	-9.020	-7.874
$S_{1v}^\dagger OS_{1v}$	14.760	8.616	0.924	0.510	1.920	1.050	0.486	0.252	9.630	6.018	3.964	2.630
$S_{1v}^\dagger OS_{2v} + cc$	8.880	5.814	0.948	0.588	2.160	1.218	-3.732	-2.640	3.342	2.940	0.941	1.124
$S_{2v}^\dagger OS_{2v}$	9.540	6.918	0.306	0.234	6.084	4.254	2.526	1.572	29.508	19.638	14.666	9.815
<i>Extra</i>		-6.408		0.030		3.366		-1.584		23.568		-15.243
<i>norm</i>	-15.276	-8.442	-0.918	-0.480	-5.952	-3.024	2.250	1.044	-34.747	-21.220	-16.646	-10.194

TABLE V: Contributions from individual LCCSD and CCSD terms to the A_{hf}/g_I calculations in the $11S$, $8D$, and $9D$ states (in MHz). *Extra* and *norm* correspond to contributions from the non-linear terms of the CCSD method that are not mentioned explicitly and corrections due to the normalization of the wave functions respectively.

CC term	$11s\ ^2S_{1/2}$		$8d\ ^2D_{3/2}$		$8d\ ^2D_{5/2}$		$9d\ ^2D_{3/2}$		$9d\ ^2D_{5/2}$	
	LCCSD	CCSD	LCCSD	CCSD	LCCSD	CCSD	LCCSD	CCSD	LCCSD	CCSD
$OT_1 + cc$	-10.583	-10.704	0.048	0.023	0.030	0.021	0.024	0.013	0.016	0.011
$T_1^\dagger OT_1$	0.150	0.154	~ 0	~ 0	~ 0	~ 0	~ 0	~ 0	~ 0	~ 0
$T_1^\dagger OT_2 + cc$	-0.429	-0.443	~ 0	~ 0	-0.001	~ 0	~ 0	~ 0	~ 0	~ 0
$T_2^\dagger OT_2$	-2.111	-2.113	0.642	0.235	0.518	0.476	0.240	0.180	0.277	0.251
$OS_{1v} + cc$	44.080	35.231	4.044	3.009	1.259	0.907	2.082	1.510	0.650	0.458
$OS_{2v} + cc$	32.902	26.513	1.290	0.831	-14.290	-11.668	0.852	0.570	-7.452	-6.095
$T_1^\dagger OS_{2v} + cc$	-0.958	-1.110	-0.072	-0.076	-0.025	-0.027	-0.036	-0.041	-0.013	-0.014
$T_2^\dagger OS_{2v} + cc$	-4.100	-4.225	0.006	0.001	0.014	0.006	0.004	0.0002	0.008	0.003
$S_{1v}^\dagger OS_{1v}$	2.610	1.667	0.456	0.253	0.121	0.063	0.222	0.118	0.060	0.030
$S_{1v}^\dagger OS_{2v} + cc$	0.819	0.776	0.894	0.553	-0.635	-0.527	0.468	0.292	-0.273	-0.220
$S_{2v}^\dagger OS_{2v}$	8.063	5.353	2.580	1.855	1.124	0.725	1.350	0.967	0.598	0.386
<i>Extra</i>		-6.099		-1.608		-0.341		-0.850		-0.210
<i>norm</i>	-8.509	-5.043	-2.352	-1.273	0.795	0.392	-1.174	-0.602	0.366	0.178

$P_{1/2}$ and $D_{3/2}$ states implying that the pair-correlation contributions are very important in all these cases. In the $P_{3/2}$ states, contributions from both these CC terms are almost same in magnitude while $OS_{2v} + cc$ are the dominant contributors in the $D_{5/2}$ states. We also find that the trends of contributions in the evaluation of B_{hf}/Q are different from those of A_{hf}/g_I . The core contributions coming through the excitation of the T operators are comparatively significant for the S - states. In general

contributions through the single core excitations (generated by T_1) are found to be important. However, there are large core contributions through the T_2 operator, particularly, for the ground state.

We list the calculated and experimental values of A_{hf} and B_{hf} for ^{210}Fr and ^{212}Fr in Table VIII for which a few high precision measurements are available. Coc et al. had obtained the A_{hf} value for the ground $7S$ state as 7195.1(4) MHz using high-resolution spectroscopy [25].

TABLE VI: Contributions from individual LCCSD and CCSD terms to the B_{hf}/Q calculations (in MHz) in the $7P_{3/2}$, $8P_{3/2}$, $6D$ and $7D$ states. *Extra* and *norm* correspond to contributions from the non-linear terms of the CCSD method that are not mentioned explicitly and corrections due to the normalization of the wave functions respectively.

CC term	$7p\ ^2P_{3/2}$		$6d\ ^2D_{3/2}$		$6d\ ^2D_{5/2}$		$8p\ ^2P_{3/2}$		$7d\ ^2D_{3/2}$		$7d\ ^2D_{5/2}$	
	LCCSD	CCSD	LCCSD	CCSD	LCCSD	CCSD	LCCSD	CCSD	LCCSD	CCSD	LCCSD	CCSD
$OT_1 + cc$	-2.237	-3.690	0.112	0.033	0.234	0.141	-0.564	-1.202	0.064	0.028	0.123	0.081
$T_1^\dagger OT_1$	0.010	0.029	~ 0	~ 0	~ 0	~ 0	0.002	0.008	~ 0	~ 0	~ 0	~ 0
$T_1^\dagger OT_2$	-0.185	-0.289	-0.001	-0.001	~ 0	-0.001	-0.051	-0.094	~ 0	~ 0	~ 0	~ 0
$T_2^\dagger OT_2$	0.692	0.888	4.559	4.332	5.157	4.926	0.364	0.248	2.409	2.060	2.530	2.162
$OS_{1v} + cc$	67.760	49.601	41.611	26.721	40.121	25.521	18.390	13.72	8.487	6.271	7.665	5.542
$OS_{2v} + cc$	103.331	88.490	26.401	39.060	55.031	68.220	31.631	27.34	5.851	10.56	14.671	19.77
$T_1^\dagger OS_{2v} + cc$	-0.434	-0.482	-0.289	-0.277	-0.306	-0.300	-0.156	-0.176	-0.109	-0.115	-0.112	-0.120
$T_2^\dagger OS_{2v} + cc$	-2.082	-1.745	-5.093	-3.812	-6.073	-4.504	-0.677	-0.576	-1.721	-1.428	-2.027	-1.652
$S_{1v}^\dagger OS_{1v}$	9.737	5.216	16.649	6.858	13.385	5.409	1.957	1.090	1.394	0.760	1.041	0.543
$S_{1v}^\dagger OS_{2v} + cc$	14.081	9.057	0.240	5.167	8.190	10.101	2.534	1.702	2.830	1.561	3.293	1.887
$S_{2v}^\dagger OS_{2v}$	-0.578	-0.436	3.294	1.293	1.873	0.595	0.153	0.103	1.620	1.015	1.472	0.954
<i>Extra</i>		-1.786		-0.006		-0.045		0.010		0.010		0.003
<i>norm</i>	-6.277	-3.312	-13.514	-7.207	-13.941	-7.415	-2.138	-1.162	-4.781	-2.961	-4.666	-2.890

TABLE VII: Contributions from individual LCCSD and CCSD terms to the B_{hf}/Q calculations (in MHz) in the $8D$ and $9D$ states. *Extra* and *norm* correspond to contributions from the non-linear terms of the CCSD method that are not mentioned explicitly and corrections due to the normalization of the wave functions respectively.

CC term	$8d\ ^2D_{3/2}$		$8d\ ^2D_{5/2}$		$9d\ ^2D_{3/2}$		$9d\ ^2D_{5/2}$	
	LCCSD	CCSD	LCCSD	CCSD	LCCSD	CCSD	LCCSD	CCSD
$OT_1 + cc$	0.035	0.017	0.065	0.044	0.019	0.010	0.036	0.024
$T_1^\dagger OT_1$	~ 0	~ 0	0.0001	0.0001	~ 0	~ 0	0.0001	~ 0
$T_1^\dagger OT_2$	-0.0001	-0.0002	-0.0001	-0.0002	-0.0001	-0.0001	~ 0	-0.0001
$T_2^\dagger OT_2$	1.214	0.992	1.262	1.035	0.653	0.523	0.677	0.545
$OS_{1v} + cc$	2.938	2.185	2.675	1.926	1.514	1.096	1.381	0.972
$OS_{2v} + cc$	2.429	4.490	6.338	8.560	1.226	2.270	3.246	4.354
$T_1^\dagger OS_{2v} + cc$	-0.051	-0.055	-0.053	-0.057	-0.028	-0.029	-0.028	-0.030
$T_2^\dagger OS_{2v} + cc$	-0.811	-0.682	-0.953	-0.786	-0.429	-0.360	-0.503	-0.415
$S_{1v}^\dagger OS_{1v}$	0.351	0.183	0.257	0.133	0.162	0.085	0.127	0.063
$S_{1v}^\dagger OS_{2v} + cc$	1.350	0.664	1.364	0.663	0.756	0.372	0.748	0.361
$S_{2v}^\dagger OS_{2v}$	0.781	0.517	0.757	0.515	0.433	0.287	0.425	0.291
<i>Extra</i>		-1.667		-1.791		-0.815		-0.871
<i>norm</i>	-1.857	-1.197	-1.801	-1.157	-0.911	-0.571	-0.865	-0.544

In the same work, Coc et al had also given A_{hf} and B_{hf} values of the $7P_{3/2}$ state as 78.0(2) MHz and 51(4) MHz respectively. Using the two-photon excitation spectroscopy of ^{210}Fr atom confined and cooled in a magneto-optical trap, Simsarian et al. had obtained the experimental A_{hf} value for the $8S$ state as 1577.8(23) MHz at the ISOLDE facility [13]. Fairly recently, Gomez et al. measured the A_{hf} value for the $9S$ state as 622.25(36) MHz using a similar experimental technique [15]. From

another experiment, Coc. et al. have reported the A_{hf} value of the $7P_{1/2}$ state as 945.6(5.8) MHz [26]. A more precise value of A_{hf} in the $7P_{1/2}$ state has been obtained by Grossman et al. as 946.6(5.8) MHz [12]. Soon after that Grossman et al. extracted the A_{hf} values for the $7D_{3/2}$ and $7D_{5/2}$ states by measuring hyperfine splittings as 22.3(5) MHz and -17.8(8) MHz respectively [14]. Here, they had neglected B_{hf} value of the $7D_{3/2}$ state while estimating a large B_{hf} value of 64(17) MHz for the

$7D_{5/2}$ state. Similarly, for the ^{212}Fr isotope there are many experimental results available for the A_{hf} and B_{hf} values measured using various spectroscopic techniques and are presented in the same Table VIII. For instance Coc et al., adopting the same experimental technique as for ^{210}Fr , have measured the A_{hf} values of the $7S$ and $7P_{1/2,3/2}$ states in ^{212}Fr [25, 26]. It can be noticed from the tabulated results for the A_{hf} values that there is excellent agreement between the present calculations with the experimental values of the $7P_{1/2,3/2}$ states whereas our results differ from the measurements by about 1.2% for the ground state. In another experiment Duong et al. had used stepwise laser excitation in collinear geometry with the on-line mass separator of the ISOLDE facility at CERN and measured the A_{hf} and B_{hf} values for the $7S$, $7P$ and $8P$ states of ^{212}Fr [27]. These experimental results are also in good agreements with our calculations for the above states. Arnold et al. had further extended this project to carry out measurements of the hyperfine structure constants of the $10S$, $11S$, $8D$ and $9D$ states in ^{212}Fr [16], which are also given in Table VIII. It can be seen that these results and our calculations agree very well.

As has been stated before, evaluation of the theoretical results for A_{hf} and B_{hf} require a knowledge of g_I (i.e. μ_I and I) and Q values of the atom. Our calculations using our CCSD $_{t3}$ method are the most rigorous theoretical results to date as they take into account more physical effects than previous calculations. The current best value of μ_I for ^{210}Fr was extracted by combining the experimental A_{hf} value of its $9S$ state with the corresponding calculation using the SDpT method [15]. However, if experimental results for hyperfine structure constants of any state are known to high precision, extraction of nuclear moments from these measurements can be justified. In reality, most of the measured A_{hf} values in ^{210}Fr are known quite precisely among which the ground state result is the most accurate (see Table VIII). To infer g_I value for ^{210}Fr from the A_{hf} results, we take the mean value from the data obtained combining the measurements with their corresponding calculations using the CCSD $_{t3}$ method for all the states except for the $D_{5/2}$ states. The reason for not considering results of these states is that the correlation effects in these cases are more than 100% while for other states the principal contributions come from the DF values. In this approach, we obtain $g_I = 0.733765942$ which corresponds to $\mu_I = 4.40(5)$ of ^{210}Fr . This value is in accordance with its earlier reported values as $\mu_I = 4.40(9)$ [28] and $\mu_I = 4.38(5)$ [15]. Unlike the case of A_{hf} , only two experimental values for B_{hf} in ^{210}Fr have been reported, among which the result for the $7D_{5/2}$ state might have been overestimated given that the wave functions of the $D_{5/2}$ states have an extremely small overlap in the nuclear region. Note that B_{hf} of the $7P_{3/2}$ state is 51(4) MHz. Thus, combining the B_{hf} value of the $7P_{3/2}$ state with the corresponding calculation, we obtain $Q = 0.196(15)b$, where the uncertainty only from

the measurement is taken into account, and the value estimated earlier was $Q = 0.19(2)b$ [28] for ^{210}Fr . The agreement between these two values is because the same experimental B_{hf} value has been used in both the results. By substituting these revised μ_I and Q values, we have evaluated the theoretical A_{hf} and B_{hf} values of ^{210}Fr and they are reported in Table VIII.

Keeping in mind the small differences among the calculations of the values of A_{hf}/g_I and B_{hf}/Q between ^{210}Fr and ^{212}Fr , as was mentioned earlier, we expect to observe the ratios between the A_{hf} and B_{hf} values from ^{210}Fr and ^{212}Fr for any given state to be almost equal to ratios of their μ_I and Q values, respectively, as per the demonstration in [29]. Considering all the experimental values known for the common states in both the isotopes, we find $g_I(^{212}\text{Fr})/g_I(^{210}\text{Fr}) = 1.25(1)$ and $Q(^{212}\text{Fr})/Q(^{210}\text{Fr}) = -0.51(5)$. Experimental results for A_{hf} and B_{hf} are reported for more states in ^{212}Fr than ^{210}Fr . Excluding A_{hf} results for the $D_{5/2}$ states owing to the reason stated previously, we obtain $g_I = 0.923070701$ for ^{212}Fr when we combine its experimental A_{hf} values of the remaining states with their respective A_{hf}/g_I calculations. This corresponds to $\mu_I(^{212}\text{Fr}) = 4.61(4)$. This, again, agrees with the previously reported value $\mu_I(^{212}\text{Fr}) = 4.62(9)$ [28]. In a similar procedure, we get $Q(^{212}\text{Fr}) = -0.10(1)b$ which is same as that given in [28]. From these theoretical results, we get $g_I(^{212}\text{Fr})/g_I(^{210}\text{Fr}) = 1.26$ and $Q(^{212}\text{Fr})/Q(^{210}\text{Fr}) \approx -0.51$, which are in reasonable agreement with the above estimated values from the measurements.

Comparison of the theoretical and experimental A_{hf} and B_{hf} results quoted in Table VIII are quite satisfactory for almost all the states, but we find a large discrepancy between the experimental and theoretical B_{hf} values in the $7D_{5/2}$ state. This result requires further theoretical and experimental verifications. Also, it was assumed that B_{hf} values of other $D_{3/2,5/2}$ states were negligible while extracting the experimental A_{hf} values of the corresponding states, however the present work shows that B_{hf} of the $7D_{3/2}$ state is about 6 MHz.

V. CONCLUSION

In summary, we have employed many-body methods at different levels of approximation to study the magnetic dipole and electric quadrupole hyperfine structure constants of the first 17 states in ^{210}Fr and ^{212}Fr . This work demonstrates the importance of the inclusion of the non-linear terms in the coupled-cluster method, that accounts for the contributions from the triples and quadrupole excitations, for the accurate evaluation of the above quantities and for the studies of the violations of parity and time reversal symmetries in Fr. By combining the experimental values with our corresponding calculations, we obtain $\mu_I = 4.40(5)$ and $Q = 0.196(15)b$ for ^{210}Fr and $\mu_I = 4.64(4)$ and $Q = 0.10(1)b$ ^{212}Fr . A reasonably good agreements between the theoretical and experimen-

TABLE VIII: Comparison between the theoretically determined and experimentally available A_{hf} and B_{hf} results (in MHz) of ^{210}Fr and ^{212}Fr .

States	^{210}Fr				^{212}Fr			
	A_{hf}		B_{hf}		A_{hf}		B_{hf}	
	Present	Experiment	Present	Experiment	Present	Experiment	Present	Experiment
$7s\ ^2S_{1/2}$	7253.45	7195.1(4) ^a			9123.72	9064.2(2) ^a 9064.4(1.5) ^b		
$7p\ ^2P_{1/2}$	938.90	945.6(5.8) ^c 946.3(2) ^d			1181.12	1189.1(4.6) ^c 1187.1(6.8) ^b 1192.0(2) ^d		
$7p\ ^2P_{3/2}$	76.52	78.0(2) ^a	50.91	51(4) ^a	96.26	97.2(1) ^a 97.2(1) ^b	-25.97	-26.0(2) ^b
$6d\ ^2D_{3/2}$	62.52		19.33		78.65		-9.86	
$6d\ ^2D_{5/2}$	-43.16		25.75		-54.30		-13.14	
$8s\ ^2S_{1/2}$	1578.99	1577.8(23) ^e			1986.13			
$8p\ ^2P_{1/2}$	294.97				371.08	373.0(1) ^b		
$8p\ ^2P_{3/2}$	25.68		16.47		32.34	32.8(1) ^b	-8.40	-7.7(9) ^b
$7d\ ^2D_{3/2}$	22.67	22.3(5) ^f	5.98	Assume 0 ^f	28.52		-3.05	
$7d\ ^2D_{5/2}$	-11.95	-17.8(8) ^f	7.82	64(17) ^f	-15.03		-3.99	
$9s\ ^2S_{1/2}$	623.50	622.25(36) ^g			784.26			
$10s\ ^2S_{1/2}$	333.32				419.27	401(5) ^h		
$8d\ ^2D_{3/2}$	10.62		2.68		13.36	13.0(6) ^h	-1.37	Assume 0 ^h
$8d\ ^2D_{5/2}$	-5.05		3.49		-6.35	-7.1(6) ^h	-1.78	-2(10) ^h
$9d\ ^2D_{3/2}$	5.77		1.42		7.26	7.1(7) ^h	-0.72	Assume 0 ^h
$9d\ ^2D_{5/2}$	-2.59		1.83		-3.25	-3.6(4) ^h	-0.94	Assume 0 ^h
$11s\ ^2S_{1/2}$	168.85				212.39	225(3) ^h		

^a[25], ^b[27], ^c[26], ^d[12], ^e[13], ^f[14], ^g[15], ^h[16].

tal results are obtained except for the electric quadrupole hyperfine structure constant of the $7D_{5/2}$ state. Theoretically predicted values for the hyperfine structure constants of many states including the $6D$ states, in the present work, could be tested experimentally in the future.

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